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Polarization of Bloch electrons and Berry phase in the presence of electromagnetic fields

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We consider Bloch electrons in the presence of the uniform electromagnetic field in two- and three-dimensions. It is renowned that the quantized Hall effect occurs in such systems. We suppose a weak and homogeneous electric field represented by the time-dependent vector potential which is changing adiabatically. The adiabatic process can be closed in the parameter space and a Berry phase is generated. In the system, one can define the macroscopic electric polarization whose time derivative is equivalent to the quantized Hall current and its conductivity is written by the Chern number. Then, the polarization is induced perpendicular to the electric field. We show that the induced polarization per a cycle in the parameter space is quantized and closely related to the Berry phase as well as the Chern number. The process is adiabatic and the system always remains the ground state, then, the polarization is quite different from the usual dielectric polarization and has some similarity to the spontaneous polarization in the crystalline dielectrics which is also written by the Berry phase. We also point out the relation between our results and the adiabatic pumping.

I. INTRODUCTION

The presence of the geometrical phase (Berry phase) was revealed in the adiabatic process of a quantum mechanical system around a closed loop in a parameter space [1]. Thus, it could be regarded as the generalization of the Aharonov-Bohm effect [2] in a parameter space. The Berry phase has been appeared in many contexts, for example, a treatment of the Born-Oppenheimer approximation [3], fractional statistics [4], the axial anomaly in field theories [5], and so on.

Recently, the relation between the spontaneous electric polarization in crystalline dielectrics and the Berry phase was discussed [6]. The authors of Ref. [6] treated the system as Bloch electrons with a finite energy gap *in the absence of* electromagnetic fields. They introduce an adiabatic change of the potential (Kohn-Sham potential) with a slowly varying parameter λ. The Hamiltonian is compactified in the parameter space, and then, a Berry phase is defined in the adiabatic process. The charge transfer occurs and the polarization is induced in this process with external electric field held to be zero, and it is represented by the Berry phase [6].

The two-dimensional (2D) Bloch electron system with an uniform magnetic field has been investigated for a long time [7], and it has been revealed that the integer quantum Hall effect occurs when the Fermi energy lies in an energy gap [8]. The integer part of the quantized Hall conductance ne^2/h ($n = 0, \pm 1, \pm 2 \cdots$) is represented by the Chern number [9,10], which is a topological number defined on the two-torus (the magnetic Brillouin zone). The effect is generalized to 3D [11,12]. Recent arguments point out that the band gap could exist for the magnetic field around 40 Tesla in organic compounds $(TMTSF)_2X$ [12,13]. Then, to realize the quantum Hall effect of Bloch electrons in 3D may be easier than that in 2D.

In this paper, we consider Bloch electrons in the presence of the uniform electromagnetic fields in 2D and 3D. A Berry phase is induced by the adiabatic change of the time-dependent vector potential. Following Ref. [6], we define the electric macroscopic polarization in the system. It is shown that the time derivative of the macroscopic electric polarization corresponds to the quantized Hall current in the system. The quantized Hall current and also the polarization is induced adiabatically. In the adiabatic process, the system always remains to be in the ground state, and then, the polarization is quite different from the usual dielectric polarization. It has been pointed out that the quantized Hall conductivity is written in terms of the Berry phase as well as the Chern number in the 2D systems [14]. Recently, the authors generalize the relation to 3D systems [15]. By using the relation between the Berry phase and the quantized Hall conductance, we can find out that the macroscopic polarization is closely related to the Berry phase. The relation between the macroscopic polarization and the Berry phase seems to be analogous to the spontaneous polarization in the crystalline dielectrics [6].

Recently, the adiabatic pumping is discussed progressively [16,17]. In pumping, an adiabatic ac perturbation yields a dc current, and the charge transfer per the cycle is independent on the period of the perturbation. We also argue the relation between our results and the adiabatic pumping.

In section II, we consider the 2D system. 3D system is discussed in section III. We set the light velocity $c = 1$ throughout the discussion.

II. MACROSCOPIC POLARIZATION AND BERRY PHASE IN 2D SYSTEM

In this section, we treat 2D noninteracting electrons in a periodic potential in the presence of a uniform magnetic field perpendicular to the plane and a uniform electric field in the plane. The electric field is represented by a time-dependent vector potential. Then we employ the adiabatic approximation assuming that the electric field is weak enough. In order to make the paper self-contained and fix the notations, we would like to introduce the discussions in Ref. [14], first. We review that the existence of the Berry phase is demonstrated in this situation and that the Chern number is written in terms of the Berry phase [14]. The Chern number is well known as a topological number which represents the integer part of the quantized Hall conductance in the system [8–10]. After these reviews, we show that the macroscopic electric polarization, whose time derivative corresponds to the Hall current in the system, is written in terms of the Berry phase.

The time-dependent Shrödinger equation we consider here is

$$i\hbar\frac{\partial\Psi(t)}{\partial t} = H(t)\Psi(t), \tag{1}$$

where

$$H(t) = \frac{1}{2m}(-i\hbar\nabla + e\mathbf{A}(t))^2 + U(\mathbf{r}),$$

and $\mathbf{A}(t)$ is the vector potential for the electromagnetic field, therefore, the magnetic field and the electric field are given by $\mathbf{B} = \nabla\times\mathbf{A}$ and $\mathbf{E} = -\partial\mathbf{A}/\partial t$, respectively. We take the Bravais lattice vectors as

$$\mathbf{R} = m\mathbf{a} + n\mathbf{b}, \tag{2}$$

where m and n are integers, and assume that the potential is periodic in both **a**- and **b**- directions, i.e.

$$U(\mathbf{r}) = U(\mathbf{r}+\mathbf{a}) = U(\mathbf{r}+\mathbf{b}). \tag{3}$$

We suppose that the electric field is weak enough. Then the system evolves slowly so that it can be described by the adiabatic approximation. At any instant, we have an eigenvalue equation

$$\begin{aligned} H(t)\Phi_n(t,\mathbf{r}) &= \left[\frac{1}{2m}(-i\hbar\nabla + e\mathbf{A}(t))^2 + U(\mathbf{r})\right]\Phi_n(t,\mathbf{r}) \\ &= E_n(t)\Phi_n(t,\mathbf{r}). \end{aligned} \tag{4}$$

The system is invariant under translations by **a** and by **b**. However, the Hamiltonian $H(t)$ is not invariant under these transformations. The reason for this is that the vector potential $\mathbf{A}(t)$ is not constant in space in spite of the fact that the magnetic field is uniform. An appropriate gauge transformation is required to make the Hamiltonian invariant. It is well known that we can construct the magnetic translation operators, which commute with Hamiltonian, written as

$$T_{\mathbf{R}} = \exp\left[i\mathbf{R}\cdot\left(-i\nabla - \frac{e}{\hbar}\mathbf{A}(t)\right)\right]. \tag{5}$$

Here we use the symmetric gauge $\mathbf{A} = (\mathbf{B}\times\mathbf{r})/2$. Now we look for eigenstates which simultaneously diagonalize $T_{\mathbf{R}}$ and H. However, note that the magnetic translations do not commute with each other in general, since

$$T_{\mathbf{a}}T_{\mathbf{b}} = \exp[2\pi i\phi]T_{\mathbf{b}}T_{\mathbf{a}}, \tag{6}$$

where $\phi = (eB/h)|\mathbf{a}\times\mathbf{b}|$ is the number of magnetic flux quanta in a unit cell. When ϕ is a rational number $\phi = p/q$ (p and q are integers with no common factor), we have a subset of translations which commute with each other. We consider the enlarged unit cell (the magnetic unit cell), in which integral magnetic flux quanta go through. For example, if we take the Bravais lattice vectors as

$$\mathbf{R}' = m\mathbf{a} + nq\mathbf{b}, \tag{7}$$

then p of the magnetic flux quanta penetrates the magnetic unit cell which is enclosed by the vectors **a** and $q\mathbf{b}$. The magnetic translation operators $T_{\mathbf{R}'}$ which corresponds to the new Bravais lattice vectors commute with each other.

Let $\Phi^{(\alpha)}$ be an simultaneous eigenfunction of the operators H and $T_{\mathbf{R}'}$, here α denotes the band index. Then the eigenvalues of $T_{\mathbf{a}}$ and $T_{q\mathbf{b}}$ are given by

$$\begin{aligned} T_{\mathbf{a}}\Phi^{(\alpha)} &= e^{i\mathbf{k}\cdot\mathbf{a}}\Phi^{(\alpha)}, \\ T_{q\mathbf{b}}\Phi^{(\alpha)} &= e^{i\mathbf{k}\cdot q\mathbf{b}}\Phi^{(\alpha)}, \end{aligned} \tag{8}$$

where $\hbar\mathbf{k}$ is the generalized crystal momentum in the magnetic Brillouin zone (MBZ). By using the primitive vectors of the reciprocal lattice

$$\begin{aligned} \mathbf{G}_a &= \frac{2\pi}{v_0}(\mathbf{b}\times\hat{\mathbf{z}}), \\ \mathbf{G}_b &= \frac{2\pi}{v_0}(\hat{\mathbf{z}}\times\mathbf{a}), \\ v_0 &= \hat{\mathbf{z}}\cdot(\mathbf{a}\times\mathbf{b}), \end{aligned} \tag{9}$$

where $\hat{\mathbf{z}}$ is the unit vector perpendicular to the 2D plane, **k** is written as

$$\begin{aligned} \mathbf{k} &= f_a\mathbf{G}_a + \frac{f_b}{q}\mathbf{G}_b \\ &0 \le f_a \le 1,\ 0 \le f_b \le 1. \end{aligned} \tag{10}$$

Therefore, the eigenfunction is labeled by **k** in addition to the band index α. For the magnetic translation invariance, we can write down the eigenfunction in the Bloch form

$$\Phi_{\mathbf{k}}^{(\alpha)}(\mathbf{r},t)=e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}^{(\alpha)}(\mathbf{r},t). \tag{11}$$

From Eq.(5) and Eq.(8), $u_{\mathbf{k}}^{(\alpha)}(\mathbf{r},t)$ should satisfy the relation

$$\begin{aligned} u_{\mathbf{k}}^{(\alpha)}(\mathbf{r}+\mathbf{a},t) &= \exp\left[i\frac{e}{\hbar}\mathbf{a}\cdot\mathbf{A}(t)\right]u_{\mathbf{k}}^{(\alpha)}(\mathbf{r},t), \\ u_{\mathbf{k}}^{(\alpha)}(\mathbf{r}+q\mathbf{b},t) &= \exp\left[i\frac{e}{\hbar}q\mathbf{b}\cdot\mathbf{A}(t)\right]u_{\mathbf{k}}^{(\alpha)}(\mathbf{r},t). \end{aligned} \tag{12}$$

This is the generalized Bloch theorem in the magnetic field [7]. The instantaneous eigenvalue equation for $u_{\mathbf{k}}^{(\alpha)}(\mathbf{r},t)$, which is obtained from Eq. (4) and Eq. (11) is written as

$$H_{\mathbf{k}}(t)u_{\mathbf{k}}^{(\alpha)}(\mathbf{r},t)=E_{\mathbf{k}}^{(\alpha)}(t)u_{\mathbf{k}}^{(\alpha)}(\mathbf{r},t), \tag{13}$$

$$H_{\mathbf{k}}(t)=\frac{(-i\hbar\nabla+\hbar\mathbf{k}+e\mathbf{A}(t))^2}{2m}+U(\mathbf{r}). \tag{14}$$

Now, we have the "Hamiltonian" $H_{\mathbf{k}}(t)$, which contains the parameters $\mathbf{k}$ and t. Note that the eigenvalue $E_{\mathbf{k}}^{(\alpha)}(t)$ depends on $\mathbf{k}$ continuously. For a fixed band index α, the set of values of $E_{\mathbf{k}}^{(\alpha)}(t)$ with $\mathbf{k}$ varying in the MBZ forms the magnetic subband.

Following Ref. [1], let us write a time-dependent wave function in the adiabatic approximation in terms of a snap shot wave function with the dynamical phase $\int_0^t dt' E_{\mathbf{k}}(t')$ and a phase $\gamma_{\mathbf{k}}^{(\alpha)}(t)$

$$\begin{aligned} \Psi_{\mathbf{k}}^{(\alpha)}(t) &= \exp\left[-\frac{i}{\hbar}\int_0^t E_{\mathbf{k}}^{\alpha}(t')dt'\right] \\ &\quad\times\exp\left[\frac{i}{\hbar}\gamma_{\mathbf{k}}^{(\alpha)}(t)\right]\Phi_{\mathbf{k}}^{(\alpha)}(t). \end{aligned} \tag{15}$$

Substitute the above form into the time-dependent Shrödinger equation Eq.(1), then, the phase $\gamma_{\mathbf{k}}^{\alpha}(t)$ is written as,

$$\begin{aligned} \gamma_{\mathbf{k}}(t) &= i\int_0^t \langle\Phi_{\mathbf{k}}(t')|\frac{d}{dt'}|\Phi_{\mathbf{k}}(t')\rangle\, dt' \\ &= i\int_0^t \langle u_{\mathbf{k}}(t')|\frac{d}{dt'}|u_{\mathbf{k}}(t')\rangle\, dt', \end{aligned} \tag{16}$$

here we omit the band index α because we will consider a single magnetic subband for a while. The "wave function" $u_{\mathbf{k}}$ obeys the "Schrödinger equation" (13).

In order to consider a Berry phase, a Hamiltonian must go around a closed loop in the parameter space in the adiabatic process. The Hamiltonian Eq. (14) as it is does not have this property. However, it is possible to compactify it as

$$H_{\mathbf{k}}(t)\sim H_{\mathbf{k}+\mathbf{G}_a}(t)\sim H_{\mathbf{k}+\mathbf{G}_b/q}(t), \tag{17}$$

where the symbol $\sim$ denotes equivalence, since we have equivalent crystal momenta and thus give the same wave function. The time-dependent part of the vector potential is written as $-\mathbf{E}t$. Suppose that the electric field is applied along $\mathbf{G}_a\perp\mathbf{b}$. Then the time-dependence of the Hamiltonian $H_{\mathbf{k}}(t)$ enters in the form $\mathbf{k}-(eEv_0t/hb)\mathbf{G}_a$. Thus we have $u_{\mathbf{k}}(t)=u_{\mathbf{k}-(eEv_0t/hb)\mathbf{G}_a}$, where $u_{\mathbf{k}}(t=0)=u_{\mathbf{k}}$, and the period of a transport around a closed path in the parameter space is given by $T=(hb/eEv_0)$ [18]. The Berry phase is obtained from Eq. (16) as

$$\begin{aligned} \Gamma_a(f_b) &= i\int_0^T \left\langle u_{\mathbf{k}-t'\frac{eEv_0}{hb}\mathbf{G}_a}\right|\frac{\partial}{\partial t'}\left|u_{\mathbf{k}-t'\frac{eEv_0}{hb}\mathbf{G}_a}\right\rangle dt' \\ &= i\int_0^1 \langle u_{\mathbf{k}}|\frac{\partial}{\partial f_a}|u_{\mathbf{k}}\rangle\, df_a, \end{aligned} \tag{18}$$

where f_a and f_b are defined in Eq. (10). $\Gamma_a(f_b)$ depends on f_b but is independent on f_a. Similarly, if the electric field is applied along $\mathbf{G}_b\perp\mathbf{a}$, we have

$$\Gamma_b(f_a)=i\int_0^1 \langle u_{\mathbf{k}}|\frac{\partial}{\partial f_b}|u_{\mathbf{k}}\rangle\, df_b. \tag{19}$$

In general, we can define T and Berry phase when the electric field is parallel to the reciprocal lattice vector for the magnetic unit cell, i.e.,

$$\mathbf{E}\ //\ (m\mathbf{G}_a+n\mathbf{G}_b/q), \tag{20}$$

where $m,n=0,\pm1,\pm2\cdots$.

Let us define a vector field in the MBZ by

$$\tilde{\mathbf{A}}(\mathbf{k})=\langle u_{\mathbf{k}}|\nabla_{\mathbf{k}}|u_{\mathbf{k}}\rangle, \tag{21}$$

where $\nabla_{\mathbf{k}}=\left[\mathbf{a}\frac{\partial}{\partial f_a}+q\mathbf{b}\frac{\partial}{\partial f_b}\right]$ is the vector operator. Then, we have

$$\Gamma_a(f_b)=i\int_0^1 df_a\mathbf{G}_a\cdot\tilde{\mathbf{A}}(\mathbf{k})=i\oint_{C(f_b)}d\mathbf{k}\cdot\tilde{\mathbf{A}}(\mathbf{k}), \tag{22}$$

where $\oint_{C(f_b)}$ denotes that the path of the line integral is taken on the closed loop where f_b is fixed. Similarly we have

$$\Gamma_b(f_a)=i\int_0^1 df_b\frac{\mathbf{G}_b}{q}\cdot\tilde{\mathbf{A}}(\mathbf{k})=i\oint_{C(f_a)}d\mathbf{k}\cdot\tilde{\mathbf{A}}(\mathbf{k}). \tag{23}$$

The vector field $\tilde{\mathbf{A}}(\mathbf{k})$ is called Berry connection. This is considered as a gauge field induced in the parameter space, or in the MBZ. Suppose $u_{\mathbf{k}}(\mathbf{r})$ satisfies the Schrödinger equation Eq. (13), then an phase transformed function

$$u'_{\mathbf{k}}(\mathbf{r})=u_{\mathbf{k}}(\mathbf{r})e^{if(\mathbf{k})}, \tag{24}$$

also satisfies Eq. (13), where $f(\mathbf{k})$ is the smooth function of $\mathbf{k}$ and is independent of $\mathbf{r}$. Under the transformation, any physical variables do not change, since this transformation is global in the coordinate space. From Eq. (21), $\tilde{\mathbf{A}}(\mathbf{k})$ is transformed as

$$\tilde{\mathbf{A}}'(\mathbf{k})=\tilde{\mathbf{A}}(\mathbf{k})+i\nabla_{\mathbf{k}}f(\mathbf{k}). \tag{25}$$

Thus, we may regard $\tilde{\mathbf{A}}(\mathbf{k})$ as a gauge field induced in the parameter space.

Let us introduce an integral

$$N_{\rm Ch} = \frac{1}{2\pi i}\int_{\rm MBZ} d^2k \left[\nabla_{\mathbf{k}} \times \tilde{\mathbf{A}}(\mathbf{k})\right]_z . \qquad (26)$$

Here, $[\cdots]_z$ expresses the z-component of the vector. The MBZ is topologically a torus T^2 rather than a rectangular in $\mathbf{k}$-space, because the points $\mathbf{k}$, $\mathbf{k}+\mathbf{G}_a$ and $\mathbf{k}+\mathbf{G}_b/q$ should be identified as equivalent points. Therefore, integral coincides with the first Chern number of a principal $U(1)$ fiber bundle on the torus T^2 whose connection is $\tilde{\mathbf{A}}(\mathbf{k})$ [9,10]. Since there are no boundary on the torus, the integral (26) becomes finite if and only if $\tilde{\mathbf{A}}(\mathbf{k})$ has non-trivial topology on the MBZ.

We apply the Stokes theorem to Eq. (26) and derive the relation between Berry phases Eqs. (22), (23) and the Chern number Eq. (26) written as [14]

$$N_{\rm Ch} = \frac{1}{2\pi}\left[\int_0^1 df_a \frac{d\Gamma_b(f_a)}{df_a} - \int_0^1 df_b \frac{d\Gamma_a(f_b)}{df_b}\right]. \qquad (27)$$

Following Ref. [6], one could define the electric contribution to the macroscopic electric polarization as,

$$\begin{aligned}\mathbf{P}(t) &= e\sum_{\alpha\le\alpha_{\rm F}}\int_{\rm MBZ}\frac{d^2k}{(2\pi)^2}\left\langle \Psi_{\mathbf{k}}^{(\alpha)}(t)\right|\mathbf{r}\left|\Psi_{\mathbf{k}}^{(\alpha)}(t)\right\rangle \\ &= e\sum_{\alpha\le\alpha_{\rm F}}\int_{\rm MBZ}\frac{d^2k}{(2\pi)^2}\left\langle u_{\mathbf{k}}^{(\alpha)}(t)\right|\mathbf{r}\left|u_{\mathbf{k}}^{(\alpha)}(t)\right\rangle, \qquad (28)\end{aligned}$$

where we use Eqs. (11) and (15), and the summation is taken over the bands below the Fermi energy. We reinstalled the band index α. The time derivative of $\mathbf{P}(t)$ is the electric current of the system. It should be the quantized Hall current when the Fermi energy lies in the gap. Actually, it is calculated as,

$$\begin{aligned}\frac{\partial \mathbf{P}(t)}{\partial t} &= e\sum_{\alpha\le\alpha_{\rm F}}\int_{\rm MBZ}\frac{d^2k}{(2\pi)^2}\left[\left\langle \frac{\partial}{\partial t}u_{\mathbf{k}}^{(\alpha)}(t)\right|\mathbf{r}\left|u_{\mathbf{k}}^{(\alpha)}(t)\right\rangle \right.\\ &\quad \left. + \left\langle u_{\mathbf{k}}^{(\alpha)}(t)\right|\mathbf{r}\left|\frac{\partial}{\partial t}u_{\mathbf{k}}^{(\alpha)}(t)\right\rangle\right] \\ &= e\sum_{\alpha\le\alpha_{\rm F}<\beta}\int_{\rm MBZ}\frac{d^2k}{(2\pi)^2}\times \\ &\quad \left[\left\langle \frac{\partial}{\partial t}u_{\mathbf{k}}^{(\alpha)}(t)\right| u_{\mathbf{k}}^{(\beta)}(t)\right\rangle\left\langle u_{\mathbf{k}}^{(\beta)}(t)\right|\mathbf{r}\left|u_{\mathbf{k}}^{(\alpha)}(t)\right\rangle \\ &\quad \left. + \left\langle u_{\mathbf{k}}^{(\alpha)}(t)\right|\mathbf{r}\left|u_{\mathbf{k}}^{(\beta)}(t)\right\rangle\left\langle u_{\mathbf{k}}^{(\beta)}(t)\left|\frac{\partial}{\partial t}u_{\mathbf{k}}^{(\alpha)}(t)\right.\right\rangle\right], \end{aligned} \qquad (29)$$

where we use the completeness condition for $|u_{\mathbf{k}}^{\beta}(t)>$

$$\sum_\beta \left|u_{\mathbf{k}}^{(\beta)}(t)\right\rangle\left\langle u_{\mathbf{k}}^{(\beta)}(t)\right| = 1,$$

and here, the summation is taken over all the bands. We can calculate the matrix element for $\alpha\neq\beta$

$$\begin{aligned}&\left\langle u_{\mathbf{k}}^{(\beta)}(t)\right|\mathbf{r}\left|u_{\mathbf{k}}^{(\alpha)}(t)\right\rangle \\ &= \frac{\left\langle u_{\mathbf{k}}^{(\beta)}(t)\right|[H(t),\mathbf{r}]\left|u_{\mathbf{k}}^{(\alpha)}(t)\right\rangle}{E_{\mathbf{k}}^{(\beta)}-E_{\mathbf{k}}^{(\alpha)}} \\ &= -i\hbar\frac{\left\langle u_{\mathbf{k}}^{(\beta)}(t)\right|\mathbf{v}(t)\left|u_{\mathbf{k}}^{(\alpha)}(t)\right\rangle}{E_{\mathbf{k}}^{(\beta)}-E_{\mathbf{k}}^{(\alpha)}} \\ &= -i\frac{\left\langle u_{\mathbf{k}}^{(\beta)}(t)\right|\partial H_{\mathbf{k}}(t)/\partial\mathbf{k}\left|u_{\mathbf{k}}^{(\alpha)}(t)\right\rangle}{E_{\mathbf{k}}^{(\beta)}-E_{\mathbf{k}}^{(\alpha)}} \\ &= -i\left\langle\frac{\partial u_{\mathbf{k}}^{(\beta)}(t)}{\partial\mathbf{k}}\right| u_{\mathbf{k}}^{(\alpha)}(t)\right\rangle \\ &= i\left\langle u_{\mathbf{k}}^{(\beta)}(t)\right|\left.\frac{\partial u_{\mathbf{k}}^{(\alpha)}(t)}{\partial\mathbf{k}}\right\rangle, \end{aligned} \qquad (30)$$

where $\mathbf{v}(t) = (-i\hbar\nabla + e\mathbf{A}(t))/m$ is the velocity operator. Then, we can find that

$$\begin{aligned}\frac{\partial\mathbf{P}}{\partial t} = ie\int_{\rm MBZ}\frac{d^2k}{(2\pi)^2}\sum_{\alpha\le\alpha_{\rm F}}\left[\left\langle\frac{u_{\mathbf{k}}^{(\alpha)}(t)}{\partial t}\right|\left.\frac{\partial u_{\mathbf{k}}^{(\alpha)}(t)}{\partial\mathbf{k}}\right\rangle - \right. \\ \left.\left\langle\frac{u_{\mathbf{k}}^{(\alpha)}(t)}{\partial\mathbf{k}}\right|\left.\frac{\partial u_{\mathbf{k}}^{(\alpha)}(t)}{\partial t}\right\rangle\right]. \end{aligned} \qquad (31)$$

We have an relation $|u_{\mathbf{k}}(t)>=|u_{\mathbf{k}-e\mathbf{E}t/\hbar}>$, thus

$$\frac{\partial u_{\mathbf{k}}(t)}{\partial t} = -\frac{e\mathbf{E}}{\hbar}\cdot\frac{\partial u_{\mathbf{k}}(t)}{\partial\mathbf{k}}.$$

Therefore, the time derivative of the macroscopic polarization is written as

$$\begin{aligned}&\frac{\partial\mathbf{P}(t)}{\partial t} \\ &= i\frac{e^2}{\hbar}\sum_{i=x,y}E_i\int_{\rm MBZ}\frac{d^2k}{(2\pi)^2}\sum_{\alpha\le\alpha_{\rm F}}\times \\ &\quad\left[\left\langle\frac{u_{\mathbf{k}}^{(\alpha)}(t)}{\partial k_i}\right|\left.\frac{\partial u_{\mathbf{k}}^{(\alpha)}(t)}{\partial\mathbf{k}}\right\rangle - \left\langle\frac{u_{\mathbf{k}}^{(\alpha)}(t)}{\partial\mathbf{k}}\right|\left.\frac{\partial u_{\mathbf{k}}^{(\alpha)}(t)}{\partial k_i}\right\rangle\right] \\ &= \frac{e^2}{h}\mathbf{E}\times\hat{\mathbf{z}}\left\{\int_{\rm MBZ}\frac{d^2k}{2\pi i}[\nabla_{\mathbf{k}}\times\tilde{\mathbf{A}}(\mathbf{k})]_z\right\} \\ &= \frac{e^2}{h}\left\{\sum_{\alpha\le\alpha_{\rm F}}N_{\rm Ch}^{(\alpha)}\right\}\mathbf{E}\times\hat{\mathbf{z}}, \end{aligned} \qquad (32)$$

where $N_{\rm Ch}^{(\alpha)}$ denotes the Chern number for the α-th band. Eq. (32) is just the quantized Hall current in the system when the Fermi energy is located between the energy gap.

Then, the polarization induced by the electric field along $\mathbf{G}_a \perp \mathbf{b}$ per the period $T = (hb/eEv_0)$ (See, the paragraph before Eq. (18)) is written as

$$
\begin{aligned}
\Delta \mathbf{P}_b &= \int_0^T dt \frac{\partial \mathbf{P}_b(t)}{\partial t} \\
&= -q\mathbf{b}\frac{e}{qv_0}\sum_{\alpha\le\alpha_{\rm F}} N_{\rm Ch}^{(\alpha)} \\
&= -q\mathbf{b}\frac{e}{qv_0}\sum_{\alpha\le\alpha_{\rm F}} \times \\
&\quad \frac{1}{2\pi}\left[\int_0^1 df_a \frac{d\Gamma_b^{(\alpha)}(f_a)}{df_a} - \int_0^1 df_b \frac{d\Gamma_a^{(\alpha)}(f_b)}{df_b}\right], \quad (33)
\end{aligned}
$$

where $\Gamma_{a,b}^{(\alpha)}$ is the Berry phase for the α-th band and we use Eq. (27). The result shows that the electric dipole moment per the magnetic unit cell is quantized as an integer multiple of $-eq\mathbf{b}$.

Similarly, when $\mathbf{E}//\mathbf{G}_b \perp \mathbf{a}$, the period $T = ha/eEqv_0$ and

$$
\Delta \mathbf{P}_a = \mathbf{a}\frac{e}{qv_0}\sum_{\alpha\le\alpha_{\rm F}} N_{\rm Ch}^{(\alpha)}. \quad (34)
$$

It is also written by the Berry phase by using Eq. (27) as well as the Chern number. The electric dipole moment per the magnetic unit cell is integer multiple of $e\mathbf{a}$.

One could point out the specific properties of the polarization in our system as follows;

(a) introduced by the *adiabatic* process

(b) perpendicular to $\mathbf{E}$

(c) written by the Berry phase

(d) independent of T, i.e. independent of $|\mathbf{E}|$

(e) the induced dipole moment per the magnetic unit cell per the period T is quantized

From (a) and (b), one can see that the polarization in our system is quite different in the usual dielectric polarization in the insulators. In the adiabatic process, the system always remains in the ground state. In insulators, the longitudinal conductivity and the translational conductivity is zero, and the charge transport would not occur adiabatically. Then, the finite polarization is obtained beyond the adiabatic approximation and the direction of the polarization is along the external electric field $\mathbf{E}$. In our system, we have a finite transverse conductivity because of the presence of the magnetic field. The transverse charge transport occurs even in the adiabatic process and the polarization is induced perpendicular to $\mathbf{E}$.

The properties (a) and (c) suggests that the polarization in our system has some similarity to the spontaneous macroscopic polarization in the crystalline dielectrics. It has been pointed out by King-Smith and Vanderbilt, and Resta [6] that the spontaneous polarization is induced by an adiabatic change of the potential (Kohn-Sham potential) with a slowly varying parameter λ. The process is defined on the closed loop in the parameter space and the Berry phase is generated, and the spontaneous polarization is written by the Berry phase. A related result is obtained in a different context [19].

We see the relation between our discussion and the adiabatic charge pumping originally argued by Thouless [16,17]. The adiabatic pumping is the charge transport whose specific properties are: (i) the adiabatic ac perturbation yields the dc current, (ii) the charge transfer does not depend on the period of the perturbation [17].

In our system, the perturbation (the electric field) itself is not ac, but the Hamiltonian $H_{\mathbf{k}}(t)$ is compactified in the parameter space and the period T is introduced, and the dc Hall current Eq. (32) flows.

The statements (d) and (e) imply the fact that the charge transfer per T across the boundary of the magnetic unit cell does not depend on T, which corresponds to the property (ii) of the adiabatic pumping, and is quantized. Actually, one can see it directly. For $\mathbf{E} \perp \mathbf{b}$, the Hall current $\partial \mathbf{P}_b/\partial t$ flows parallel to $\mathbf{b}$ and across the boundary a-axis. The normal vector of the boundary is $\mathbf{G}_a/|\mathbf{G}_a|$. Then, the charge transfer is

$$
\begin{aligned}
\Delta Q &= \int_0^T dt \int_0^1 df_a \frac{\mathbf{G}_a}{|\mathbf{G}_a|}\cdot\frac{\partial \mathbf{P}_b}{\partial t} \\
&= \int_0^1 df_a \frac{\mathbf{G}_a}{|\mathbf{G}_a|}\cdot \Delta \mathbf{P}_b \\
&= -e\sum_{\alpha\le\alpha_{\rm F}} N_{\rm Ch}^{(\alpha)}. \quad (35)
\end{aligned}
$$

For $\mathbf{E} \perp \mathbf{a}$, the charge transfer is

$$
\Delta Q = e\sum_{\alpha\le\alpha_{\rm F}} N_{\rm Ch}^{(\alpha)}. \quad (36)
$$

Similar results are obtained by Thouless for the commensurate periodic ac perturbation [16]. The commensurability seems to correspond to the direction of $\mathbf{E}$ in our discussion (See. Eq. (20)), which is essential to define T and ΔQ.

III. MACROSCOPIC POLARIZATION AND BERRY PHASE IN 3D SYSTEM

The aim of this section is to argue the 3D generalization of the discussions in the previous section. We define the macroscopic polarization. One can see that its time derivative is equivalent to the quantized Hall current in 3D. The Hall conductivity is represented by the Chern number and quantized when the Fermi energy lies on the band gap [11]. Recent arguments point out that such a gap could exist for the magnetic field around 40 Tesla in organic compounds $(TMTSF)_2X$ [12,13]. Then, it may

be easier to realize the quantum Hall effect of Bloch electrons in 3D rather than 2D. Our discussion written below could be applicable to such compounds by using the tight-binding scheme.

The relation between the Berry phase and the Chern number is also driven in the system [15]. Then, we would find out the relation between the macroscopic polarization and the Berry phase in 3D system as well as 2D system. We also point out the relation between our results and the adiabatic pumping [16,17].

Let us consider the 3D Bloch electrons in the presence of uniform electromagnetic fields. We have a periodic potential $U(\mathbf{r}) = U(\mathbf{r}+l\mathbf{a}+m\mathbf{b}+n\mathbf{c})$ (l, m, n; integers). The electric field we consider here is weak and described by an adiabatically changing vector potential. We use the adiabatic approximation and first, we consider the eigenstates of the Hamiltonian $H(t)$ at fixed t.

We have a magnetic field written as,

$$\mathbf{B} = B_a\mathbf{a} + B_b\mathbf{b} + B_c\mathbf{c}, \tag{37}$$

where $\mathbf{a}, \mathbf{b}$ and $\mathbf{c}$ are the primitive vectors for the Bravais lattice. Let $\mathbf{G}_a = (2\pi/v_0)(\mathbf{b}\times\mathbf{c})$, $\mathbf{G}_b = (2\pi/v_0)(\mathbf{c}\times\mathbf{a})$ and $\mathbf{G}_c = (2\pi/v_0)(\mathbf{a}\times\mathbf{b})$ stand for the fundamental reciprocal lattice vectors, where $v_0 = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})$. B_a, B_b and B_c are written as,

$$\begin{aligned} B_a &= \frac{1}{2\pi}\mathbf{B}\cdot\mathbf{G}_a = \frac{1}{v_0}\frac{h}{e}\phi_a, \\ B_b &= \frac{1}{2\pi}\mathbf{B}\cdot\mathbf{G}_b = \frac{1}{v_0}\frac{h}{e}\phi_b, \\ B_c &= \frac{1}{2\pi}\mathbf{B}\cdot\mathbf{G}_c = \frac{1}{v_0}\frac{h}{e}\phi_c, \end{aligned} \tag{38}$$

where ϕ_a, ϕ_b and ϕ_c is a number of the unit flux through the plane $\mathbf{b}\times\mathbf{c}$, $\mathbf{c}\times\mathbf{a}$ and $\mathbf{a}\times\mathbf{b}$, respectively. We introduce a "rational magnetic fields", where $\phi_a = p_a/q_a$, $\phi_b = p_b/q_b$ and $\phi_c = p_c/q_c$ are rational values. Here p_i, and q_i ($i = a, b, c$) are the integers without common factor. Let q stands for the least multiple factor for the three integers q_a, q_b and q_c. We can write $\phi_a = N_a/q$, $\phi_b = N_b/q$ and $\phi_c = N_c/q$ (N_i; integer, $i = a, b, c$). Let p stands for the largest common factor for three integers N_a, N_b and N_c. The magnetic field is written as

$$\begin{aligned} \mathbf{B} &= \frac{1}{v_0}\frac{h}{e}\frac{p}{q}\mathbf{c}', \\ \mathbf{c}' &= (n_a\mathbf{a} + n_b\mathbf{b} + n_c\mathbf{c}). \end{aligned} \tag{39}$$

By definition, n_a, n_b and n_c are integers with no common factor. It means that there are no vectors on the Bravais lattice which is the submultiple of $\mathbf{c}'$, and it was shown by Ref. [11] that we can find vectors $\mathbf{a}'$ and $\mathbf{b}'$ such that $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{c}'$ are a new set of primitive vectors as follows. Let r stands for the greatest common factor of n_c and n_a. Therefore, there is no common factor of r and n_b. Then we can choose four integers s_a, s_b, s_c and s_r, which satisfy relations

$$s_a n_a + s_c n_c = r,\ \ s_b n_b + s_r r = 1,$$

and we may choose

$$\begin{aligned} \mathbf{a}' &= s_c\mathbf{a} - s_a\mathbf{c}, \\ \mathbf{b}' &= s_r\mathbf{b} - \frac{s_b n_c}{r}\mathbf{c} - \frac{s_b n_a}{r}\mathbf{a}. \end{aligned}$$

The Hamiltonian has the magnetic translation symmetry. Actually, we can choose the magnetic unit cell with the primitive vectors $\mathbf{a}'$, $q\mathbf{b}'$ and $\mathbf{c}'$, and the magnetic translation operators for the Bravais lattice

$$\mathbf{R}' = l\mathbf{a}' + mq\mathbf{b}' + n\mathbf{c}' \quad (l, m, n;\ \text{integer}),$$

is written by the 3D generalization of Eq. (5) when we take the symmetric gauge. Three operators $T_{\mathbf{a}'}$, $T_{q\mathbf{b}'}$ and $T_{\mathbf{c}'}$ commute with the Hamiltonian at any instant, and also with each other. The wavevector in the magnetic Brillouin zone (MBZ) is written as

$$\mathbf{k} = f_{a'}\mathbf{G}_{a'} + \frac{f_{b'}}{q}\mathbf{G}_{b'} + f_{c'}\mathbf{G}_{c'},\ \ 0 < f_{a'}, f_{b'}, f_{c'} < 1. \tag{40}$$

Then, the eigenstates of the Hamiltonian at any instant is the generalized Bloch states. The Bloch wave function with a band index α is written as $\Phi^{\alpha}_{\mathbf{k}}(\mathbf{r},t) = e^{i\mathbf{k}\cdot\mathbf{r}}u^{(\alpha)}_{\mathbf{k}}(\mathbf{r},t)$, where $u^{\alpha}_{\mathbf{k}}(\mathbf{r},t)$ satisfies

$$\begin{aligned} &H_{\mathbf{k}}(t)u^{(\alpha)}_{\mathbf{k}}(t,\mathbf{r}) \\ &= \left[\frac{1}{2m}(-i\nabla + \mathbf{k} + e\mathbf{A}(t))^2 + U(\mathbf{r})\right]u^{(\alpha)}_{\mathbf{k}}(t,\mathbf{r}) \\ &= E^{(\alpha)}_{\mathbf{k}}(t)u^{(\alpha)}_{\mathbf{k}}(t,\mathbf{r}), \\ &\mathbf{A}(t) = -\mathbf{E}t + \frac{1}{2}\mathbf{B}\times\mathbf{r}, \end{aligned} \tag{41}$$

which is the 3D generalization of Eqs. (13) and (14). The function $u^{(\alpha)}_{\mathbf{k}}(\mathbf{r},t)$ has relations in the symmetric gauge:

$$\begin{aligned} u^{(\alpha)}_{\mathbf{k}}(\mathbf{r}+\mathbf{a}',t) &= \exp\left[i\frac{e}{\hbar}\mathbf{a}'\cdot\mathbf{A}(t)\right]u^{(\alpha)}_{\mathbf{k}}(\mathbf{r},t), \\ u^{(\alpha)}_{\mathbf{k}}(\mathbf{r}+q\mathbf{b}',t) &= \exp\left[i\frac{e}{\hbar}q\mathbf{b}'\cdot\mathbf{A}(t)\right]u^{(\alpha)}_{\mathbf{k}}(\mathbf{r},t), \\ u^{(\alpha)}_{\mathbf{k}}(\mathbf{r}+\mathbf{c}',t) &= \exp\left[i\frac{e}{\hbar}\mathbf{c}'\cdot\mathbf{A}(t)\right]u^{(\alpha)}_{\mathbf{k}}(\mathbf{r},t). \end{aligned} \tag{42}$$

As well as 2D, we have a relation

$$u^{(\alpha)}_{\mathbf{k}}(t) = u^{(\alpha)}_{\mathbf{k}-t\frac{e\mathbf{E}}{\hbar}}. \tag{43}$$

According to Berry [1], in the adiabatic approach, the solution for the time-dependent Shrödinger equation $i\hbar\partial\Psi(t)/\partial t = H(t)\Psi(t)$ can be written with a phase $\gamma^{(\alpha)}_{\mathbf{k}}(t)$ as

$$\Psi_{\mathbf{k}}^{(\alpha)}(t,\mathbf{r}) = \exp\left[-i\int_0^t dt' E_{\mathbf{k}}^{(\alpha)}(t')\right] \times \exp\left[i\gamma_{\mathbf{k}}^{(\alpha)}(t)\right] e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}^{(\alpha)}(t,\mathbf{r}). \tag{44}$$

We will discuss the presence of the Berry phase later, and first, we show the time derivative of the macroscopic polarization is equivalent to the quantized Hall current in 3D [11] as follows. The polarization is defined by the 3D generalization of Eq. (28). The definition agrees with that in Ref. [6]. Generalizing the derivation of Eq. (32) to 3D case, we obtain the equation

$$\frac{\partial \mathbf{P}}{\partial t} = \frac{e^2}{2\pi h}\mathbf{E}\times\mathbf{D}, \quad \mathbf{D} = \frac{1}{2\pi i}\sum_{\alpha\le\alpha_{\mathrm{F}}}\int_{\mathrm{MBZ}} d^3k[\nabla_{\mathbf{k}}\times\tilde{\mathbf{A}}^{(\alpha)}(\mathbf{k})], \tag{45}$$

where we introduce a "gauge field" defined as $\tilde{\mathbf{A}}^{(\alpha)}(\mathbf{k}) = \left\langle u_{\mathbf{k}}^{(\alpha)}|\nabla_{\mathbf{k}}|u_{\mathbf{k}}^{(\alpha)}\right\rangle$, which is the 3D extension of Eq. (25). What we have to do here is to investigate the form for the three dimensional vector $\mathbf{D}$. We expand $\mathbf{D}$ by the fundamental reciprocal vectors $\mathbf{G}_{a'}$, $\mathbf{G}_{b'}$ and $\mathbf{G}_{c'}$. The coefficient of the vector $\mathbf{G}_{c'}$ is written as

$$t_{c'} = \frac{1}{2\pi}(\mathbf{c}'\cdot\mathbf{D}) = \sum_{\alpha\le\alpha_{\mathrm{F}}}\int_0^1 df_3\int_{S(f_3)}\frac{d^2k}{2\pi i}\left[\nabla_{\mathbf{k}}\times\tilde{\mathbf{A}}^{(\alpha)}(\mathbf{k})\right]\cdot\frac{\mathbf{c}'}{|\mathbf{c}'|}. \tag{46}$$

Here, we use the relation $\int_{MBZ} d^3k = \int_0^1 df_3(\mathbf{G}_{c'}\cdot\mathbf{c}'/|\mathbf{c}'|)\int_{S(f_3)} d^2k$, where $S(f_3)$ denotes the plane between two fundamental reciprocal vectors $\mathbf{G}_{a'}$ and $\mathbf{G}_{b'}$ (See, Eq. (40)). The r.h.s. of Eq. (46) is essentially equivalent to the Chern number [9–11]. We can show in the same manner that $t_{a'} = \mathbf{a}'\cdot\mathbf{D}/2\pi$ and $t_{b'} = q(\mathbf{b}'\cdot\mathbf{D})/2\pi$ are also equivalent to the Chern number. Because of the topological nature, these three numbers $t_{a'}$ $t_{b'}$ and $t_{c'}$ become integer whenever the Fermi energy lies in the energy Gap, even if the magnetic field is not rational. By choosing a different MBZ, in which the roles of $\mathbf{a}'$ and $\mathbf{b}'$ are exchanged, we can find that $\mathbf{b}'\cdot\mathbf{D}/2\pi$ is itself an integer. Therefore, $\mathbf{D}$ is a vector on the reciprocal lattice generated by $\mathbf{G}_{a'}$, $\mathbf{G}_{b'}$ and $\mathbf{G}_{c'}$ written as

$$\mathbf{D} = \mathbf{G} = -(t_{a'}\mathbf{G}_{a'} + t_{b'}\mathbf{G}_{b'} + t_{c'}\mathbf{G}_{c'}), \tag{47}$$

i.e.

$$\frac{\partial \mathbf{P}(t)}{\partial t} = \frac{e^2}{2\pi h}\mathbf{E}\times\mathbf{G}. \tag{48}$$

Eq. (47) and (48) suggest that $\partial\mathbf{P}/\partial t$ is actually the quantized Hall current in 3D [11].

Then, we will derive the relation between the Berry phase and the Chern number in 3D. This is the 3D generalization of the discussion in Ref. [14]. Recently, the calculation is noted by the authors [15].

By substituting Eq. (44) into the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\Psi_{\mathbf{k}}^{(\alpha)}(t)}{\partial t} = H(t)\Psi_{\mathbf{k}}^{(\alpha)}(t),$$

$\gamma_{\mathbf{k}}^{\alpha}(t)$ is obtained as

$$\gamma_{\mathbf{k}}^{(\alpha)}(t) = i\int_0^t dt'\left\langle u_{\mathbf{k}}^{(\alpha)}(t')\left|\frac{\partial}{\partial t'}\right|u_{\mathbf{k}}^{(\alpha)}(t')\right\rangle = i\int_0^t dt'\left\langle u_{\mathbf{k}-e\mathbf{E}t'/\hbar}^{(\alpha)}\left|\frac{\partial}{\partial t'}\right|u_{\mathbf{k}-e\mathbf{E}t'/\hbar}^{(\alpha)}\right\rangle. \tag{49}$$

In order to consider the Berry phase, a Hamiltonian must go around a closed loop in a parameter space in adiabatic process. The Hamiltonian $H_{\mathbf{k}}(t)$ as it is not have this property. However, it is possible to compactify it into the magnetic Brillouin zone as $H_{f_1+1,f_2,f_3}(t) \sim H_{f_1,f_2+1,f_3}(t) \sim H_{f_1,f_2,f_3+1}(t) \sim H_{f_1,f_2,f_3}(t)$, where f_1, f_2 and f_3 parameterizes $\mathbf{k}$ as Eq. (40) [18]. Repeating the discussions in 2D system and by using Eq. (21), Berry phases in the case that $\mathbf{E}//\mathbf{G}_{a'}$, $\mathbf{E}//\mathbf{G}_{b'}$ and $\mathbf{E}//\mathbf{G}_{c'}$, are written as

$$\Gamma_{a'}^{(\alpha)}(f_{b'},f_{c'}) = i\oint_{C(f_{b'},f_{c'})} d\mathbf{k}\cdot\tilde{\mathbf{A}}^{(\alpha)}(\mathbf{k}) = i\int_0^1 df_{a'}\mathbf{G}_{a'}\cdot\tilde{\mathbf{A}}^{(\alpha)}(\mathbf{k}), \tag{50}$$

$$\Gamma_{b'}^{(\alpha)}(f_{c'},f_{a'}) = i\oint_{C(f_{c'},f_{a'})} d\mathbf{k}\cdot\tilde{\mathbf{A}}^{(\alpha)}(\mathbf{k}) = i\int_0^1 \frac{df_{b'}}{Q}\mathbf{G}_{b'}\cdot\tilde{\mathbf{A}}^{(\alpha)}(\mathbf{k}), \tag{51}$$

and

$$\Gamma_{c'}^{(\alpha)}(f_{a'},f_{b'}) = i\oint_{C(f_{a'},f_{b'})} d\mathbf{k}\cdot\tilde{\mathbf{A}}^{(\alpha)}(\mathbf{k}) = i\int_0^1 df_{c'}\mathbf{G}_{c'}\cdot\tilde{\mathbf{A}}^{(\alpha)}(\mathbf{k}), \tag{52}$$

respectively. Here, $\oint_{C(f_i,f_j)}$, $(i,j = a',b',c')$ denotes that the path of the line integral is taken on a loop where parameters f_i and f_j are fixed. In general, we can define the Berry phase when the electric field is parallel to the reciprocal lattice vector for the magnetic unit cell, i.e.,

$$\mathbf{E}\ //\ (l\mathbf{G}_a + m\mathbf{G}_b/q + n\mathbf{G}_c), \tag{53}$$

where $l,m,n = 0,\pm1,\pm2\cdots$.

We apply the Stokes theorem in Eq. (46) and one of the three integers $t_{c'}$, which is equivalent to the Chern number, can also be written in terms of Berry phase as

$$t_{c'} = \frac{1}{2\pi}\sum_{\alpha\le\alpha_{\rm F}}\int_0^1 df_{c'}\left[\int_0^1 df_{a'}\frac{d}{df_{a'}}\Gamma^{(\alpha)}_{b'}(f_{c'},f_{a'}) - \int_0^1 df_{b'}\frac{d}{df_{b'}}\Gamma^{(\alpha)}_{a'}(f_{b'},f_{c'})\right], \tag{54}$$

and also $t_{a'}$, $t_{b'}$ are written as

$$t_{a'} = \frac{1}{2\pi}\sum_{\alpha\le\alpha_{\rm F}}\int_0^1 df_{a'}\left[\int_0^1 df_{b'}\frac{d}{df_{b'}}\Gamma^{(\alpha)}_{c'}(f_{a'},f_{b'}) - \int_0^1 df_{c'}\frac{d}{df_{c'}}\Gamma^{(\alpha)}_{b'}(f_{c'},f_{a'})\right], \tag{55}$$

$$t_{b'} = \frac{1}{2\pi}\sum_{\alpha\le\alpha_{\rm F}}\int_0^1 df_{b'}\left[\int_0^1 df_{c'}\frac{d}{df_{c'}}\Gamma^{(\alpha)}_{a'}(f_{b'},f_{c'}) - \int_0^1 df_{a'}\frac{d}{df_{a'}}\Gamma^{(\alpha)}_{c'}(f_{a'},f_{b'})\right]. \tag{56}$$

Then, we calculate the macroscopic polarization change per a cycle. As well as 2D, we can define the cycle when $\mathbf{E}$ is parallel to the reciprocal lattice vector $l\mathbf{G}_a + m\mathbf{G}_b + n\mathbf{G}_c$. For example, the period is written as (See, the paragraph before Eq. (18)),

$$T = \begin{cases} \frac{h}{v_0}\frac{|\mathbf{b}'\times\mathbf{c}'|}{eE} \text{ for } \mathbf{E}//\mathbf{G}_{a'} \perp b'c' - \text{plane}, \\ \frac{h}{qv_0}\frac{|\mathbf{c}'\times\mathbf{a}'|}{eE} \text{ for } \mathbf{E}//\mathbf{G}_{b'} \perp c'a' - \text{plane}, \\ \frac{h}{v_0}\frac{|\mathbf{a}'\times\mathbf{b}'|}{eE} \text{ for } \mathbf{E}//\mathbf{G}_{c'} \perp a'b' - \text{plane}. \end{cases} \tag{57}$$

Then, the polarization change per T is given;

$$\Delta\mathbf{P} = \begin{cases} \frac{e}{qv_0}(q\mathbf{b}'t_{c'} - \mathbf{c}'qt_{b'}) \text{ for } \mathbf{E} \perp b'c' - \text{plane}, \\ \frac{e}{qv_0}(\mathbf{c}'t_{a'} - \mathbf{a}'t_{c'}) \text{ for } \mathbf{E} \perp c'a' - \text{plane}, \\ \frac{h}{qv_0}(\mathbf{a}'qt_{b'} - q\mathbf{b}'t_{a'}) \text{ for } \mathbf{E} \perp a'b' - \text{plane}. \end{cases} \tag{58}$$

For Eqs. (54),(55) and (56), the polarization is written in terms of the Berry phase. The dipole moment per the magnetic unit cell i.e. $qv_0\Delta\mathbf{P}$ is quantized in each cases.

Therefore, one can see that the polarization in 3D also has the properties (a), (b), (c), (d), and (e) written in the previous section. Then, the polarization is quite different from the usual dielectric polarization and has similarity with the spontaneous polarization in dielectric crystalline [6]. As a property that it is absent in 2D, one can point out that the polarization changes its direction discretely in the 2D plane perpendicular to $\mathbf{E}$, when one changes the location of the Fermi level. The fact reflects the feature of the 3D quantized Hall effect [11].

As well as 2D, the quantization of the dipole moment per the magnetic unit cell per T implies the quantized charge transfer across the boundary of the magnetic unit cell per T. As the simple extension of Eq. (35) to 3D, one can obtain the charge transfer

$$\Delta Q = \begin{cases} -e(qt_{b'} - t_{c'}) \text{ for } \mathbf{E} \perp b'c' - \text{plane}, \\ -e(t_{c'} - t_{a'}) \text{ for } \mathbf{E} \perp c'a' - \text{plane}, \\ -e(t_{a'} - qt_{b'}) \text{ for } \mathbf{E} \perp a'b' - \text{plane}. \end{cases} \tag{59}$$

We should note the fact that the charge transfer is caused by the dc Hall current and the results does not depend on T. Then, the results is similar to the adiabatic pumping with the commensurate periodic ac perturbation [16]. The commensurability seems to correspond to the direction of $\mathbf{E}$ in our discussion (See. Eq. (53)), which is essential to define T and ΔQ.

IV. SUMMARY

In this paper, we have considered Bloch electrons in the presence of uniform electromagnetic fields in 2D and 3D. The Berry phase has been induced by the adiabatic change of the time-dependent vector potential. Following Ref. [6], the electric macroscopic polarization has been defined in the system. It has been shown that the time derivative of the macroscopic electric polarization corresponds to the quantized Hall current in the system whose conductivity is represented by the Chern number. Recently, it was shown that the Hall conductivity is written by the Berry phase as well as the Chern number in the 2D systems [14], and also in 3D systems [15]. Then, we have found out that the macroscopic polarization is closely related to the Berry phase. The quantized Hall current and also the polarization has been induced adiabatically. In the adiabatic process, the system always remains in the ground state, and then, the polarization in our system is quite different from the usual dielectric polarization. The relation between the macroscopic polarization and the Berry phase is analogous to that between the spontaneous polarization in the crystalline dielectrics and the Berry phase [6]. We have also argued the relation between our results and the adiabatic pumping, which is discussed progressively [16,17].

We have discussed the analogy among the polarization in the quantum Hall system, the spontaneous polarization in dielectric crystalline and the adiabatic pumping. As an essential point, the analogy comes from the fact that these effects are caused by the closed adiabatic change in the Bloch electron systems with the finite energy gap.

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